Resonance-induced effects in photonic crystals

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Abstract

For the case of a simple face-centered-cubic photonic crystal of homogeneous dielectric spheres, we examine to what extent single-sphere Mie resonance frequencies are related to band gaps and whether the width of a gap can be enlarged due to nearby resonances. Contrary to some suggestions, no spectacular effects may be expected. When the dielectric constant of the spheres ε_s is greater than the dielectric constant ε_b of the background medium, then for any filling fraction f there exists a critical ε_c above which the lowest lying Mie resonance frequency falls inside the lowest stop gap in the (111) crystal direction, close to its midgap frequency. If $\varepsilon_s < \varepsilon_b$, the correspondence between Mie resonances and both the (111) stop gap and a full gap does not follow such a regular pattern. If the Mie resonance frequency is close to a gap edge, one can observe a resonance-induced widening of a relative gap width by $\approx 5\%$.

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I. INTRODUCTION

Photonic crystals, i.e., dielectrics with spatial periodicity, have triggered much interest recently [1–4]. One can picture a photonic crystal as a periodic arrangement of dielectric scatterers. For example, its dielectric constant $\varepsilon(\mathbf{r})$ equals ε_s for $\mathbf{r}$ inside the scatterer and ε_b otherwise. Similarly to the case of an electron moving in a periodic potential, a photon traveling in a photonic crystal encounters a periodicaly changing dielectric constant. As a result, a gap can open in the electromagnetic wave spectrum, independent of its polarization and direction of propagation [3,4]. In a given frequency interval the density of states (DOS) can either be reduced down to zero (photonic band gap) or enhaced with respect to its vacuum value. Such a change in the DOS affects many physical quantities. The most transparent is the change in the spontaneous emission (SE) rate of embedded atoms and molecules. This can be demonstrated already at a relatively low refractive index contrast (≈ 1.15) [5]. Suppression of the SE may have applications for semiconductor lasers, solar cells, heterojunction bipolar transistors, and thresholdless lasers [1]. On the other hand, the enhancement of the SE is a way to create new sources of light for ultra-fast optical communication systems [6]. Unlike conventional (electronic) crystals, photonic crystals are essentially man-made structures and their parameters can be changed at will. There is a common belief that in the near future such systems will allow us to perform many functions with light that ordinary crystals do with electrons.

Thus far, the main emphasis in the study of photonic crystals has been on calculating the band structure [3,7–9]. Let f be the scatterer filling fraction, i.e., the volume of the scatterer(s) in the unit cell per unit cell volume. Once f is fixed, the spectrum is only a function of the dielectric contrast $\delta = \max(\varepsilon_s/\varepsilon_b, \varepsilon_b/\varepsilon_s)$. In our paper we pose the question of to what extent the single sphere resonance frequencies are related to band gaps, whether a gap width can be enlarged due to nearby resonances, and what other effects, if any, single-scatterer resonances may have on the band structure and properties of a photonic crystal.

In the following, we focus on the case of a simple face-centered-cubic (fcc) photonic crystal of homogeneous spheres. There are at least two reasons to consider this case. Firstly, single-sphere resonances, known also as Mie resonances [10], are well understood and an analytic solution exists for them. In each angular-momentum channel characterized by the angular-momentum number l a single sphere has an infinite number of Mie's resonances. The properties of Mie's resonances are discussed in many monographs (see, for example, [11]) and we only emphasize the following ones. The sharpness of a Mie resonance decreases with increasing σr_s, where r_s is the sphere radius, $\sigma = \omega\sqrt{\varepsilon_b}/c$, ω is the frequency, and c is the speed of light in vacuum. On the other hand, reflecting the centrifugal barrier increasing with l as $l(l+1)$, the sharpness increases with l. The spacing between resonances in the higher frequency range is accounted for by the resonance condition $\sigma r_s = m\pi/2$, where m is an integer (if $\varepsilon_b = 1$).

Secondly, fcc structures of homogeneous spheres are among the most promising candidates to achieve a full photonic gap at optical and near-infrared frequencies. Indeed, in this frequency range one often uses collodial systems of microspheres which can self-assemble into three-dimensional fcc crystals with excellent long-range periodicity [12,13]. This long-range periodicity gives rise to the strong optical Bragg scattering, clearly visible by the naked eye, and already described in 1963 [14]. Both the case of "dense" spheres ($\varepsilon_s > \varepsilon_b$) [13] and "air"

spheres ($\varepsilon_s < \varepsilon_b$) [15] can be realized experimentally.

The outline of our paper is as follows. In the next section, main features of the method that is used to calculate the spectrum of electromagnetic waves in periodic structures are discussed. We also discuss the differences between and similarities of the electronic and electromagnetic bands and give their rough classification. In section III we summarize our numerical results on the effects induced by resonant scattering in a simple fcc crystal of dielectric spheres. Contrary to the suggestions made previously in the literature [2], no spectacular effects may be expected. Finally, in section IV our conclusions are presented.

II. RESONANCE SCATTERING AND BAND STRUCTURE OF PHOTONIC CRYSTALS

Multiple scattering of classical waves in the presence of resonant scatterers was first studied in a disordered medium. There resonances cause a scattering delay due to the storage of wave energy inside a single scatterer, resulting in a sharp decrease (depending on the filling fraction) of the transport velocity v_E of light [16]. The discussion of resonance-induced effects in an ordered medium has been initiated by John [2]. He suggested that the coinciding resonance and Bragg scattering is the most favourable condition for opening a gap in the spectrum. In the case of spheres this leads to $f = 1/(2\sqrt{\delta})$ [2]. Later on, Zhang and Satpathy [17] noticed that a pseudogap in the band structure of an fcc lattice of dense spheres corresponds to a Mie resonance. Recently, Ohtaka and Tanabe [18], using the KKR method described earlier in [22], made an attempt to relate the Mie resonances to the photonic bands. They paid attention to flat bands which correspond to "heavy photons" in analogy to their electronic analogue, heavy fermions. For heavy photons, the group velocity can be as low as $\sim c/100$ [18]. The role of Mie resonances in bonding of spheres in photonic crystals was investigated by Antonoyiannakis and Pendry [19].

In our paper, we shall attempt to investigate the complementary relation to that discussed by Ohtaka and Tanabe [18], namely, to what extent the single sphere resonance frequencies are related to band *gaps*, a question asked first by John [2]. In obtaining his result, John [2] used a simplified picture in which, regardless of the propagation and polarization, the photon always encounters precisely the same periodic $\varepsilon(\mathbf{r})$ variation, resulting in a one-dimensional Kronig-Penney's (KP) model [20]. However, this approximation is only partially justified in the short-wavelength limit when light in a sphere behaves like a field in a slab with thickness $2r_s$. For real crystals the situation is different and the above coincidence condition can only be met in restricted regions on the surface of the Brillouin zone. Also, with increasing dielectric contrast δ, dispersion curves $\omega = \omega(\mathbf{k})$ become nonlinear and the diffraction condition is modified as compared to the Bragg case and fulfilled at lower frequency [13]. Moreover, the model neglects polarization dependent effects.

However, it is quite difficult to relax the simplifying assumptions of the one-dimensional KP model [20] made by John [2]. In our discussion of resonance-induced effects in photonic crystals we shall employ the machinery of the on-shell multiple-scattering theory (MST) (see [21] for electrons and [22] for photons). Note that the on-shell MST is already required in the one-dimensional KP model if one wants to go beyond the dispersion relation and obtain Green's function or the local density of states [23]. The unique feature of the on-

shell MST is that, for nonoverlapping (muffin-tin) scatterers [21,24] (the present situation), it disentangles single-scattering and multiple-scattering effects (see [25] for a recent discussion). For example, the total T-matrix per unit cell can be written in the form [21,22,24,26]

$$T = 1/(R^{-1} - B) = R/(1 - BR). \tag{1}$$

Here all quantities are ordinary matrices. R stands for the on-shell reaction matrix (also known as the k-matrix [24]) of the scattering sphere (of all scatterers inside the lattice unit cell in the case of a complex lattice). It is diagonal in the angular-momentum basis and can be written as $R_{LL'} = -\delta_{LL'} \tan \eta_L / \sigma$, where η_L is a phase shift. Here L is a composite index which labels all the spherical harmonics in the irreducible representation of the rotation group characterized by the principal angular-momentum number l and, in the case of electromagnetic waves, it carries an additional polarization dependent index [22]. $B = B(\sigma, \mathbf{k})$ in Eq. (1) is a matrix of so-called structure constants which accounts for the periodicity of the lattice. It depends on σ and the Bloch momentum $\mathbf{k}$. The R-matrix is singular at Mie resonance frequencies and $B(\sigma, \mathbf{k})$ is singular whenever $\sigma^2 = (\mathbf{k} + \mathbf{K}_n)^2$, where $\mathbf{K}_n$ is a vector of the dual lattice.

The exact eigenmodes of a crystal are determined by poles of the total T-matrix, the latter being the zeros of the determinant of a hermitian matrix $R^{-1} - B$,

$$\det(R^{-1} - B) = 0. \tag{2}$$

Equation (2) is the familiar Korringa-Kohn-Rostocker (KKR) equation [27] in band structure theory. Recently, we have succesfully used this approach to calculate the band structure of electromagnetic waves in a simple fcc lattice of dielectric spheres [9], to establish a simple analytic formula describing the width of the lowest lying stop gap in the (111) crystal direction (the L point of the Brillouin zone [28]) [29], and to calculate the properties of the local DOS in one dimension [23]. In general, the higher frequency, the higher the value of l_{max} is needed to ensure convergence. In order to reproduce the first band and the linear part of the spectrum, $l_{max} = 1$ is enough. In general, the size of a secular equation is reduced by almost a factor 10 compared with that in the plane-wave method [3,7,8,17] which customarily requires well above a thousand plane waves. The precision of the elements of the secular equation is determined by the standard Ewald summation [27] which yields structure constants up to six digits.

At first sight, there seem to be large differences in band formation between the electrons and electromagnetic waves. In the case of electrons, in the medium between two atoms, waves are evanescent in nature, while electromagnetic wave propagates unattenuated between two scatteres. However, electrons are strongly interacting with each other. If the interactions are taken into account, an effective-Hamiltonian single-electron picture emerges of a near-free electron with a positive energy which moves unattenuated between two scatteres like the electromagnetic wave does [26]. Therefore, the same principles apply to the classification of the electronic and the photonic bands. For electrons, a rough classification of the bands can be obtained if the singularities of R and B are well separated [26]. Thus if $R(\sigma)$ is sufficiently small near a singularity of $B(\sigma, \mathbf{k})$, where $\sigma = \sqrt{E}$ and E is the electron energy, a band is formed with the dispersion relation

$$\omega(\mathbf{k}) \approx |\mathbf{k} + \mathbf{K}_n| + R(\sigma). \tag{3}$$

In more intuitive terms, the formation of such a band results from the formation of standing waves in a crystal and it is appropriate to call such a band the Bragg band. The second type of band can form near a singularity of R at ω_0, $R = \Gamma/(\omega^2 - \omega_0^2)$. This is, for example, the case in the transition and noble metals. If Γ and $B(\sigma, \mathbf{k})$ in the vicinity of ω_0 are *sufficiently* small, a (usually very narrow) resonance band is formed with the dispersion relation [26]

$$\omega(\mathbf{k}) \approx [\omega_0 + \Gamma B(\sigma_0, \mathbf{k})]^{1/2}. \tag{4}$$

Eq. (4) is in agreement with the observation made in [18] that the resonance-band width is *comparable* with the lifetime broadening of the DOS profile for a single sphere. In more intuitive terms, formation of the resonance band can be understood as resulting from the broadening of individual resonances when they start to feel the presence of each other, similar to the formation of the electronic bands from individual atomic levels in the tight-binding limit [26]. Such usually very narrow resonance bands describe "heavy photons".

This shows that one can associate with a resonance a (resonance) band. Is it possible to associate with a resonance a gap? The answer is yes. However, a hybridization of bands must take place. We speak of hybridization if the singularities of R and B cannot be well separated and neither a pure Bragg nor a pure resonance band is formed. Under certain conditions the two bands can hybridize in such a way as to create a gap over the approximate energy range of the original unhybridized resonance band. An example of such a hybridization is provided by transition metals with characteristic d (or f) resonance which couples with extended band states by tunneling [30]. In the latter case a broad $s - p$ band hybridizes with a narrow d band in such a way as to create a gap over the approximate energy range of the original unhybridized d resonance band [30].

In the following section, we investigate the hybridization of photonic bands in an fcc lattice of dielectric spheres. Although the same principles apply to the classification of the photonic bands as to those for electrons, is does not mean that the respective band structures are qualitatively similar. There is significantly difficult to open a gap in the spectrum of electromagnetic waves than in the case of electrons. Moreover, a gap often does not open between the lowest lying bands, as in the case of electrons, but in an intermediate region. The origin of this difference lies in a different behaviour of R and B and can be rather easily understood. Indeed, in the tight-binding picture of band formation [26], individual bands results from the broadening of corresponding atomic levels when the atoms start to feel the presence of each other. The largest gap between atomic levels is between the lowest-lying energy levels. Therefore, for a lattice of atoms, one expects to find a gap essentially between the first and the second energy band, with the gap between higher bands scaling down to zero. On the other hand, for a dielectric scatterer and Maxwell's equations, bound states are absent. They are replaced by resonances. Moreover, if the wavelength is small compared to the size of the spheres, one can use geometric optics, while in the opposite limit of long wavelengths, the Rayleigh approximation applies. In neither case does a gap open in the spectrum. Therefore, if a gap is present in the spectrum, it should be in the intermediate region between the two limiting cases (see, however, the case of a diamond lattice ([3], figure 2), which is a complex lattice). The same applies to the localization of light [2] which is also expected at some intermediate frequencies.

Since opening of a gap in the spectrum of electromagnetic waves in much difficult than

in the electronic case, one expects also that hybridization will be weaker in the former case. These expectations are confirmed in the following section.

III. RESULTS FOR AN FCC LATTICE OF DIELECTRIC SPHERES

In our case of an fcc crystal of homogeneous spheres, we looked for a correspondence between Mie resonance frequencies and (i) the lowest lying stop gap in the (111) crystal direction (the L point of the Brillouin zone [28]) in the case of both "dense" spheres ($\varepsilon_s > \varepsilon_b$) and "air" spheres ($\varepsilon_s < \varepsilon_b$), (ii) the full gap in the case of "air" spheres. (Note that there is no full gap in the case of "dense" spheres [7,9].) Apart from numerous experimental data now available [13,31], there are at least two other reasons to chose the L-gap. First, the width of the first stop gap often takes on its maximum at the L point and, second, experimental techniques make it possible to grow collodial crystals such that the L direction corresponds to normal incidence on the crystal surface.

In the case of "dense" spheres we found that for sufficiently high dielectric contrast δ the L-gap can be associated with the 1M1 resonance. (Our notation lAn for a Mie resonance is such that l is the angular momentum, A stands for either electric (E) or magnetic (M) mode, and n is the order of the resonance with increasing frequency in a given lA channel.) For all filling fractions one finds that as δ increases over a critical value (see Figure 1), the 1M1 resonance "descends" from above to the L-gap and stays inside it close to the midgap frequency. We verified this behaviour for δ up to 100.

In the case of "air" spheres the hybridization of bands is much less pronounced compared to the case of "dense" spheres. We observe a correspondence between the L-gap and a Mie resonance only for particular filling fractions and dielectric contrasts. Filling fraction $f \approx 0.5$ or higher is required for hybridization to occur. However, for a given f, the required dielectric contrast for the onset of hybridization can be as little as half the value for the dense sphere case. For $f = 0.6$ one finds the 1E1 resonance trapped inside the L-gap already for $\delta \geq 8$. In the close-packed case the lowest lying 1E1 resonance descends actually below the L-gap and, if $\delta \geq 16$, a hybridization occurs at the frequency corresponding to the second, 1M1, resonance.

Hybridization in the case of the lowest L-gap is only partial since the gap does not extend over the whole Brillouin zone. Let us, therefore, look at the full band gap which can be opened only in the air sphere case (one can open just a single full gap here [7,9]). In contrast to that of the L-gap, the opening of the full gap requires a certain threshold dielectric contrast which rapidly increases as f decreases from the close-packed case [7,9] (see figure 2). Hybridization follows the irregular pattern seen in the case of the L-gap. For example, for $f = 0.6$ hybridization occurs if $\delta \geq 36$ where the 2M1 resonance descends from above to the full gap, soon followed by the 3E1 resonance (2M1 < 3E1). Both resonances seem to be locked inside the full gap (at least up to $\delta = 100$). Interesting behaviour is found for $f = 0.64$. First, the full gap opens at $\delta \approx 10.6$ between the closely lying 2M1 and 3E1 resonances. As ε_b increases, the 3E1 resonance moves across the gap and stays closely below the lower edge of the full gap. Hybridization around the 3E1 resonance occurs only for $\delta = (11.5, 13)$. Outside this interval of δ no resonance is inside the full gap. The case in which $f = 0.68$ shows an anomalous behaviour: no resonance frequency is inside the full gap

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or close to the the full gap edge. On the other hand, in the close-packed case ($f \approx 0.74$) one can find three closely lying resonances, namely, 3M1, 4E1, and 1E2 (3M1 < 4E1 < 1E2), inside the full gap. 3M1 descends to the full gap around $\varepsilon_b = 12$, soon followed by the 4E1 and 1E2 resonances. For $\varepsilon_b > 16$ all three resonances are already inside the full gap and seem to remain trapped there (at least up to $\varepsilon_b = 100$).

Apart from the hybridization, another intriguing issue is that of whether the width of a gap can be enlarged due to the Mie resonances as the one-dimensional KP model suggests [2]. Once a resonance was inside a gap we did not find any significant effect on the gap width. A good illustration of this is the behaviour of the relative width Δ^r of the full gap (the full gap width divided by the midgap frequency) at $f = 0.68$ on the one hand and $f = 0.6$, 0.64 and 0.74 (close-packed) on the other hand (see figure 2). In the first case, the gap does not correspond to any Mie resonance, while in the second case, there are up to three Mie resonances inside the gap. Had there been some effect of a Mie resonance on the gap width, one would have observed either a sudden increase in Δ^r after hybridization sets in, or an anomalously small gap width for $f = 0.64$ (if $\delta > 13$) and $f = 0.68$. Instead, one sees a monotonical increase of Δ^r as δ and f increase. However, something different may happen if a Mie resonance frequency is close to a gap edge, before hybridization sets in. Under certain circumstances one can observe a resonance-induced widening of a relative gap width by up to 5%. Figure 3 shows the relative L-gap width Δ_L^r for air spheres and $f = 0.6$. Around $\delta = 7.99$ the 1E1 resonance crosses the upper edge of the L-gap, which results in a local enhancement of Δ_L^r by $\approx 5\%$. As a function of δ, this widening occurs within the very narrow interval of $\delta \in (7.986, 7.998)$ where it shows a flat peak. In the air-sphere case one can be sure that this widening of a gap can be entirely attributed to a resonance. As shown recently [29], the lowest lying L-gap for an fcc lattice of dielectric spheres can be understood in terms of simple quantities, namely, the volume averaged dielectric constant, $\bar{\varepsilon} = f\varepsilon_s + (1-f)\varepsilon_b$, the volume averaged $\varepsilon^2(\mathbf{r})$, $\overline{\varepsilon^2} = [f\varepsilon_s^2 + (1-f)\varepsilon_b^2]$, and the effective dielectric constant ε_{eff}. The effective dielectric constant can be well approximated [9,32] by Maxwell-Garnett's formula [33],

$$\varepsilon_{eff} \approx \varepsilon_b \, (1 + 2\,f\alpha)/(1 - f\alpha) \tag{5}$$

where, for a homogeneous sphere, the polarizability factor

$$\alpha = (\varepsilon_s - \varepsilon_b)/(\varepsilon_s + 2\varepsilon_b). \tag{6}$$

Then the absolute L-gap width $\triangle_L$ is approximated within 3-6% (depending on f) by the formula [29]

$$\triangle_L = C(f) \left(\sqrt{\overline{\varepsilon^2}} - \varepsilon_{eff} \right)^{1/2} \bigg/ \bar{\varepsilon} \tag{7}$$

where

$$C(f) = C_0 + 0.14 \, f \, (2f_m - f)/f_m^2. \tag{8}$$

Here $C_0 \approx 0.74$ is the minimal value of C and f_m is the filling fraction for which $C(f)$ takes on its maximal value. $C(f)$ takes on its minimal value C_0 at the extreme filling fractions

$f = 0$ and $f = 0.74$, and its maximal value is $C_m \approx 0.88$ at $f_m \approx 0.74/2$. The factor 0.14 in the interpolation formula (8) is the difference $C_m - C_0$. Let k_L be the length of the Bloch vector at the L point of the Brillouin zone. In units where the length of the side of the conventional unit cell of the cubic lattice is $A = 2$, one has $k_L/\pi = \sqrt{0.75}$. The formula

$$\triangle_L^r = 2\pi n_{eff} \triangle_L / k_L \tag{9}$$

then describes $\triangle_L^r$ for $1 \leq \delta \leq 100$ with the relative error ranging from $\approx 4\%$ for f around 0.2, to the relative error $\approx 8\%$ for the close-packed case. Formula (9) describes Δ_L^r in the air sphere case irrespective whether there is ($f \geq 0.5$) or is not ($f < 0.5$) a Mie resonance within the L-gap frequencies. However, the formula is violated in the narrow interval $\delta \in (7.986, 7.998)$ where the local widening of Δ_L^r takes place.

IV. CONCLUSION

Using the photonic analog of the KKR method [9,22], we have investigated Mie-resonance-induced effects for an ordered medium, namely, for a simple fcc lattice of homogeneous spheres in three dimensions. Our work partially fills the gap in the understanding of resonance-induced effects compared to a disordered medium [16]. We showed that the same principles apply to the classification of both electronic and electromagnetic bands in a periodic medium, although their respective qualitative behaviour may be different. For example, due to the absence of bound states for a single scatterer, it is much more difficult to open a full gap in the spectrum of electromagnetic waves than for the case of electrons. Still, under certain conditions, one can identify a resonance band, and a hybridization of the Bragg and resonance bands can take place, leaving behind a gap over the approximate energy range of the original unhybridized resonance band [30]. We investigated both a partial hybridization in the case of the first stop gap in the (111) crystal direction (the L-gap) and a full hybridization in the case of the full band gap. For dense spheres ($\varepsilon_s > \varepsilon_b$), partial hybridization around the lowest Mie resonance occurs for all filling fractions f, once the dielectric contrast δ reaches a critical value $\delta_c(f)$ (see Figure 1). For air spheres ($\varepsilon_s < \varepsilon_b$), the hybridization follows an irregular pattern and it can be observed only if $f \geq 0.5$. However, the value $\delta_c(f)$ can be as little as half the corresponding $\delta_c(f)$ in the dense-sphere case. Near close packing ($f \approx 0.74$), the partial hybridization occurs around the second Mie resonance. The full hybridization in the case of air spheres (there is no full gap in the dense sphere case [7–9]) follows again the irregular pattern seen in the case of partial hybridization. Sometimes the full gap opens in a frequency region which does not correspond to any Mie resonance ($f = 0.68$), but in other situations there are up to three Mie resonances in the frequency range corresponding to the full gap ($f = 0.74$). The resonant-induced widening of a gap can occur if a Mie resonance is about to cross the edge of the gap (see Figure 3). The values of the dielectric contrast required to observe some of these effects are within experimental reach at microwaves and, in the air-sphere case, even at optical and near-infrared frequencies. However, unlike in the case of the one dimensional Kronig-Penney model [2], we did not find any evidence that if some of Mie resonance frequencies fall inside a gap, then this leads to its significant widening. Contrary to the suggestions made previously in the literature [2], no spectacular effects may be expected. This is probably related to the

known fact that the hybridization of bands in higher dimensions is weaker [30]. Also, since the opening of a gap in the spectrum of electromagnetic waves in much difficult than in the electronic case, it is natural that also hybridization effects are weaker in the photonic case.

V. ACKNOWLEDGEMENT

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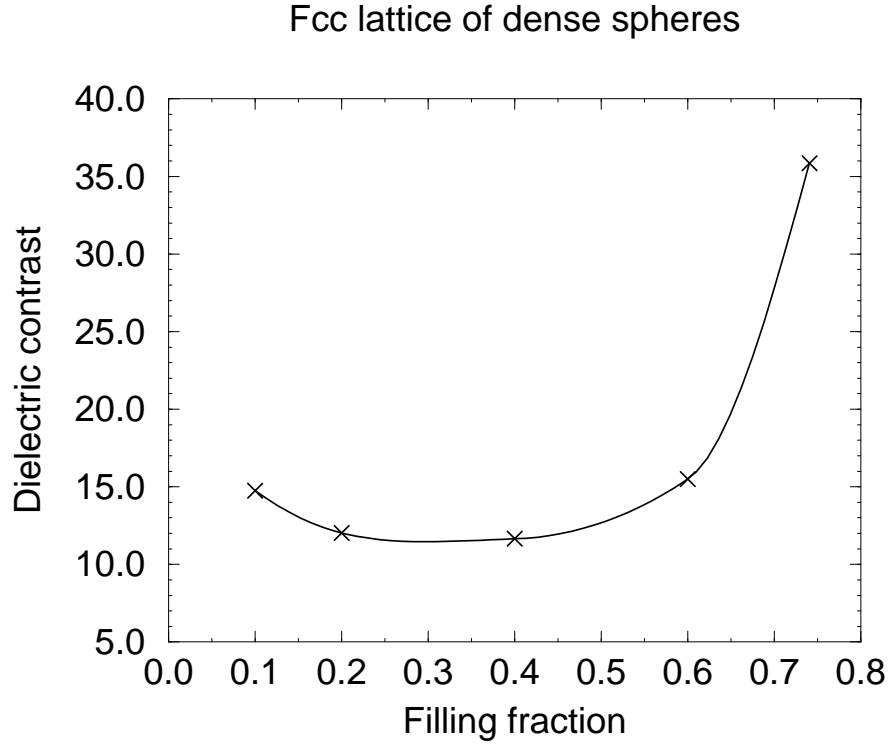
Fcc lattice of dense spheres

FIG. 1. The value of the dielectric contrast at which the lowest Mie resonance enters the L gap versus filling fraction in the case of an fcc lattice of homogeneous dense spheres.
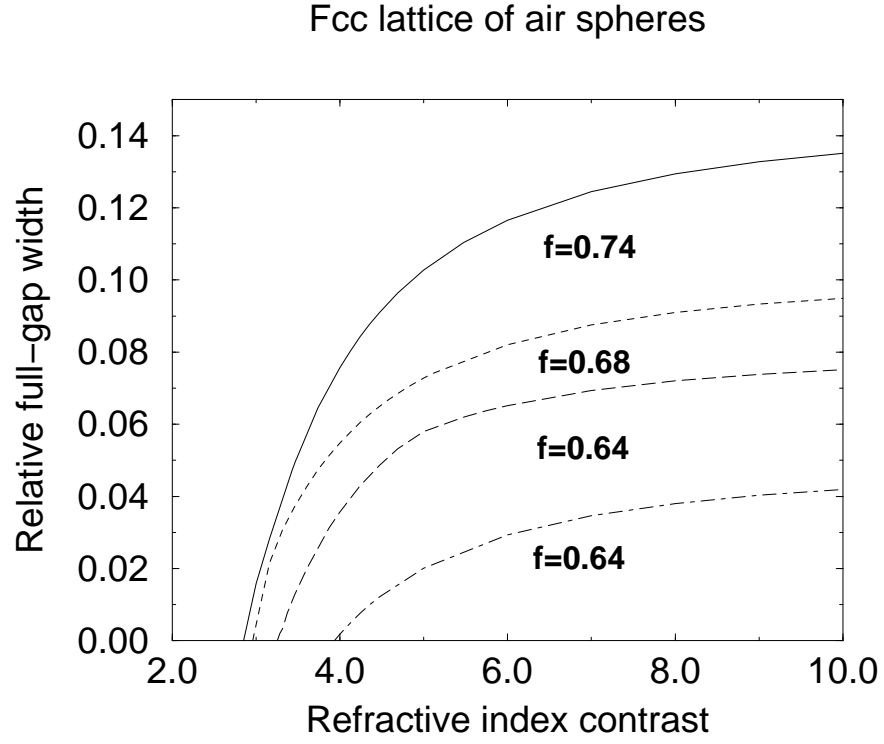
Fcc lattice of air spheres

FIG. 2. The relative width Δ^r of the full gap (the full gap width divided by the midgap frequency) in the case of an fcc lattice of homogeneous air spheres as a function of the refractive index contrast $\sqrt{\delta}$ for different filling fractions f.
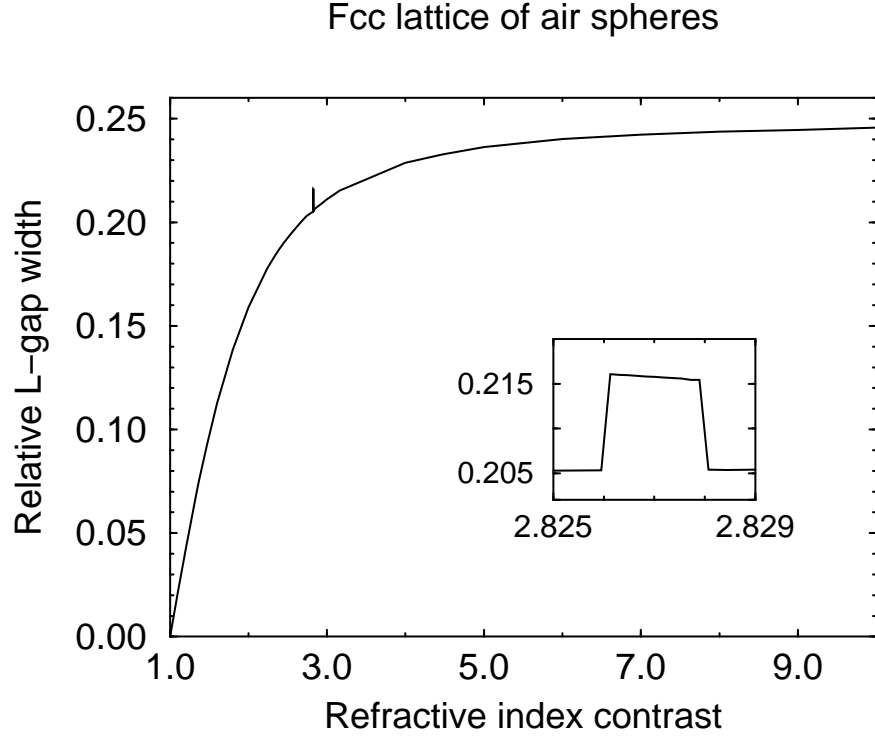
Fcc lattice of air spheres

FIG. 3. The relative L-gap width Δ_L^r (the L-gap width divided by the midgap frequency) for an fcc lattice of air spheres with the sphere filling fraction $f = 0.6$ plotted against the refractive index contrast $\sqrt{\delta}$. Around $\delta = 7.99$, the 1E1 resonance crosses the upper edge of the L-gap which results in a local enhancement of the relative L-gap width, which is shown as a very narrow peak in the main figure. The inset shows the detailed view of the peak.